Nonperturbative Dynamical Theory and A Scheme for Nonequilibrium Transport

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(Dated: February 6, 2008)

We develop a nonperturbative dynamical theory (NDT) that is useful for treating nonequilibrium transport in a system with strong correlation. We apply our NDT to the single-impurity Anderson model in equilibrium to check its reliability by comparing with the results of numerical renormalization group method (NRG). We finally suggest a self-consistent loop to calculate the current in a lead-dot-lead system with Kondo coupling.

One of the most problematic subjects in the field of theoretical condensed matter physics is the treatment of nonequilibrium transport[1] in a system with strong correlation. There is no established theory for treating the interacting system when it approaches nonequilibrium state, and a strongly correlated system requires nonperturbative treatment. Moreover, methods based on the static nonperturbative theory, such as NRG[2, 3], are inappropriate for studying nonequilibrium transport, because current is a dynamical quantity. Therefore, a possible method for the treatment of nonequilibrium transport in a system with strong correlation is by employing the NDT, which has not been studied successfully thus far. Here, we report an NDT that is developed by fully utilizing the dynamical nature of the Heisenberg picture. We first apply the new NDT to the single-impurity Anderson model in equilibrium; further, we extend the application to the nonequilibrium transport of a lead-dot-lead system.

Transport phenomena in mesoscopic systems have recently attracted considerable interest in connection with nonequilibrium transport in a strongly correlated system, which is one of challenging and debated subjects in recent theoretical condensed matter physics. An example of a typical quantum system with strong correlation under nonequilibrium conditions is a quantum dot with metallic leads under bias. Theoretical studies on quantum dot have usually reported the conductance properties that can be obtained by using the NRG, since conductance is an equilibrium property of the system. Even though the NRG has been successful in providing low-energy eigenvalues and eigenstates rigorously for a part of strongly correlated systems, it cannot be a resolver of the nonequilibrium transport problem.

A good formalism for nonequilibrium transport has been established by Meir and Wingreen[4] in terms of nonequilibrium Green's functions. Let us consider the motion of a spin-up electron in a quantum dot under bias. Since the movement of a spin-up electron will be affected by the movement of the spin-down electron due to strong correlation at the dot, the retarded on-site Green's function of a spin-up electron must contain information on the back and forth movement of the spin-down electron. A static theory such as NRG is incapable of yielding information on the back and forth movement of an electron with a particular spin. A dynamical theory, however, can incorporate this information in Green's function. In this work, we present an NDT giving the nonequilibrium Green's function that can provide a spectral density for the Anderson model when the system is in equilibrium, which is comparable to the one obtained by the NRG, and a scheme providing the current-voltage characteristics under nonequilibrium conditions.

The Heisenberg picture stresses the dynamics of operators compared with other two pictures. However, the advantage of its dynamical nature has not received sufficient appreciation. Here, we focus on the dynamical nature of the Heisenberg picture to develop the NDT. The formal solution of the Heisenberg equation for a fermion annihilation operator $c_{d\uparrow}$, i.e., $c_{d\uparrow}(t) = c_{d\uparrow} + [\hat{H}, c_{d\uparrow}](it) + [\hat{H}, [\hat{H}, c_{d\uparrow}]](it)^2/2 + \cdots$, where $\hat{H}$ is the Hamiltonian of the system, describes the time evolution of $c_{d\uparrow}$. The operators in each term of the expansion represent linearly independent ways of annihilation of a spin-up electron at site d at time t. These operators provide linearly independent bases spanning the operator or Liouville space. We call these the dynamical bases. The inner product in the Liouville space is defined as $\langle \hat{A}|\hat{B}\rangle \equiv \langle\{\hat{A}, \hat{B}^\dagger\}\rangle$, where $\hat{A}$ and $\hat{B}$ are elements of the Liouville space, the curly brackets denote the anticommutator, and the angular brackets indicates an equilibrium or nonequilibrium average, depending on the situation. Constructing appropriate dynamical bases is the essence of the NDT.

We first develop our NDT for the single-impurity Anderson model represented by the Hamiltonian $\hat{H} = \sum_\sigma \epsilon_d c^\dagger_{d\sigma} c_{d\sigma} + \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma}(V_{kd} c^\dagger_{d\sigma} c_{k\sigma} + V^*_{kd} c^\dagger_{k\sigma} c_{d\sigma}) + U n_{d\uparrow} n_{d\downarrow}$, where $n_{d\downarrow} = c^\dagger_{d\downarrow} c_{d\downarrow}$, and the subscripts σ, k, and d denote the spin index, quantum state of the metallic reservoir, and the position of impurity, respectively, and then compare the result for the spectral density with that of the NRG. Finally, we apply our NDT to study the nonequilibrium transport of the lead-dot-lead system with on-site Coulomb interaction.

The basis operators created by the commutators with the Hamiltonian are composed of $c_{k\uparrow}$ where $k = d, 1, 2, \cdots, \infty$ and the operators combined with $c_{k\uparrow}$ and other operators such as $n_{d\downarrow}$, $j^-_{d\downarrow}$, and $j^+_{d\downarrow}$, where $j^-_{d\downarrow} = i[\hat{H}, n_{d\downarrow}] = i(\sum_k V_{kd} c^\dagger_{k\downarrow} c_{d\downarrow} - \sum_k V^*_{kd} c^\dagger_{d\downarrow} c_{k\downarrow})$, i.e., the current operator, and $j^+_{d\downarrow} = i[n_{d\downarrow}, j^-_{d\downarrow}] = (\sum_k V_{kd} c^\dagger_{k\downarrow} c_{d\downarrow} +$

FIG. 1: Pictorial descriptions of the roles of basis operators $n_{d\downarrow}c_{k\uparrow}$ (a) and $j^{\mp}_{d\downarrow}c_{d\uparrow}$ for a particular $\mathbf{k}$-state (b). Sum over all $\mathbf{k}$ in (b) becomes $j^{\mp}_{d\downarrow}c_{d\uparrow}$. The dashed arrows do not indicate hybridization. They just indicate creation and annihilation.

$\sum_k V^*_{kd}c^\dagger_{d\downarrow}c_{k\downarrow}$). We keep the meaningful operators that describe the virtual exchange between spin-up and spin-down electron and take the mean-field approximation for other part of the primitive basis operator. After this manipulation, appropriate linearly independent dynamical bases spanning a reduced Liouville space of the operator $c_{d\uparrow}$ can be constructed. The bases except $c_{d\uparrow}$ itself must be orthogonal to $c_{d\uparrow}$ in order to yield a correct projection $\langle\{c^\dagger_{d\uparrow}, c_{d\uparrow}(t)\}\rangle$ that gives the on-site retarded Green's function.

The dynamical bases of the reduced Liouville space of $c_{d\uparrow}$ are composed of five parts. The first two are (i) a set of bases S_k defined by $S_k = \{c_{k\uparrow}|k = 1, 2, \cdots, \infty\}$ for describing the annihilation at the impurity site after some hoppings in the metal and (ii) a set of bases S_n defined by $S_n = \{\delta n_{d\downarrow}c_{k\uparrow}|k = 1, 2, \cdots, \infty\}$ where $\delta n_{d\downarrow} = n_{d\downarrow} - \langle n_{d\downarrow}\rangle$ for describing the number fluctuation of the spin-down electron at the impurity site during the annihilation process of (i). Lastly, we consider the bases coupled to $c_{d\uparrow}$, i.e., (iii) a set of bases S_d defined by $S_d = \{c_{d\uparrow}, \delta j^-_{d\downarrow}c_{d\uparrow}, \delta j^+_{d\downarrow}c_{d\uparrow}\}$ for describing the annihilation of a spin-up electron at the impurity site without any coupled processes and with the processes coupled to the back and forth fluctuation of the spin-down electron at the impurity site. The latter describes the hybridization in the Kondo process.

The bases of the first subset S_k and $c_{d\uparrow}$ constitute a complete set when the system is noninteracting. Since $\delta n^2_{d\downarrow}$ is composed of a constant and $\delta n_{d\downarrow}$, the first two subsets, S_k and S_n, along with $c_{d\uparrow}$, contain all the dynamical processes described by number fluctuations of a spin-down electron during the annihilation process of a spin-up electron at site d. The operators in the third subset, $\delta j^{\pm}_{d\downarrow}c_{d\uparrow}$, contribute to describing the Kondo effect. As an example, the pictorial descriptions of the basis operators $\delta n_{d\downarrow}c_{k\uparrow}$ and $\delta j^{\pm}_{d\downarrow}c_{d\uparrow}$ are shown in Fig. 1. We do not consider the other complicated processes that can occur during the annihilation process of a spin-up electron at time t since the processes considered above may be sufficient for describing the Kondo phenomena in the single-impurity Anderson model. In addition, the operator $c_{d\uparrow}$ is orthogonal to all other bases of the reduced Liouville space.

We are now in a position to obtain the spectral density of a spin-up electron at site d by NDT using the dynamical bases introduced above. The resolvent Green's function operator in the Heisenberg picture is written as $\hat{G}^{\pm} = (\omega \pm i\eta - \mathbf{L})^{-1}$, where $\mathbf{L}$ is the Liouville operator defined by $\mathbf{L}\hat{A} = \hat{H}\hat{A} - \hat{A}\hat{H}$, η is a positive infinitesimal, and the superscripts $\pm$ denote retarded $(+)$ and advanced $(-)$, respectively. This expression becomes $\hat{G}^{\pm} = (\omega \pm i\eta - \hat{H})^{-1}$ in the Schrödinger picture.

Since the retarded and advanced Green's functions are given by $G^{\pm}_{ij}(\omega) = \langle\hat{e}_i|(\omega \pm i\eta - \mathbf{L})^{-1}|\hat{e}_j\rangle$, where $|\hat{e}_j\rangle$ is one of basis operators spanning the Liouville space, they are given by the inverse of the matrix $\mathbf{M}$ defined by $\mathbf{M}_{ji} = \langle\hat{e}_i|z\mathbf{I} + i\mathbf{L}|\hat{e}_j\rangle$, where $z = -i\omega \pm \eta$, i.e., $iG^{\pm}_{ij}(\omega) = \langle\hat{e}_i|\mathbf{M}^{-1}|\hat{e}_j\rangle = (\text{adj }\mathbf{M})_{ij}[\det\mathbf{M}]^{-1}$, where $(\text{adj }\mathbf{M})_{ij}$ denotes the cofactor of the ji-element in the determinant of $\mathbf{M}$[5]. This expression has also been reported in literature[6].

In constructing matrix $\mathbf{M}$, we use normalized bases in order to make it quasi-symmetrical. If we arrange S_k, S_n, and S_d in a regular sequence to construct the matrix $\mathbf{M}$ for the single-impurity Anderson model, it is represented by a matrix of four blocks,

$$\mathbf{M}_{\text{SIAM}} = \begin{pmatrix} \mathbf{M}_r & \mathbf{M}_{dr} \\ -\mathbf{M}^*_{dr} & \mathbf{M}_d \end{pmatrix},$$

where the subindex r represents metallic reservoir. The blocks $\mathbf{M}_r$, $\mathbf{M}_{dr}$, and $\mathbf{M}_d$ are $\infty\times\infty$, $3\times\infty$, and 3×3 matrices, respectively. Since the inner product has a relation $\langle i\mathbf{L}\hat{A}|\hat{B}\rangle = -\langle i\mathbf{L}\hat{B}|\hat{A}\rangle^*$, only the real parts of the matrix elements have different signs for their counterparts.

The block $\mathbf{M}_r$ is represented by

$$\mathbf{M}_r = \begin{bmatrix} \mathbf{M}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_{11} \end{bmatrix},$$

where $\mathbf{M}_{11}$ is diagonal and its elements are $z + i\epsilon_k$, $k = 1, 2, \cdots, \infty$. The $3\times\infty$ block $\mathbf{M}_{dr}$, on the other hand, has the form

$$\mathbf{M}_{dr} = \begin{bmatrix} \mathbf{C_{kd}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C_{nj^-}} & \mathbf{C_{nj^+}} \end{bmatrix},$$

where the column $\mathbf{C_{kd}}$ has iV_{kd} as its elements, while $\mathbf{C_{nj^-}}$ and $\mathbf{C_{nj^+}}$ have $\xi^-_d V_{kd}$ and $\xi^+_d V_{kd}$, respectively. The blocks except $\mathbf{M}_d$ contribute to the self-energy. The 11-element of the block $\mathbf{M}_d$ is $z + i(\epsilon_d + \langle n_{d\downarrow}\rangle U)$, and the other diagonal elements are given by $z + i\epsilon_d + [U\langle n_{d\downarrow}\delta j^{\mp 2}_{d\downarrow}\rangle/\langle\delta j^{\mp 2}_{d\downarrow}\rangle]$. These are equal to the 11-element of $\mathbf{M}_d$ under the decoupling approximation. The off-diagonal elements of $\mathbf{M}_d$, on the other hand, are given by $\mathrm{M}^{12}_d = -\mathrm{M}^{21}_d = (U/2)\xi^-_d$, $\mathrm{M}^{13}_d = -\mathrm{M}^{31}_d = (U/2)\xi^+_d$,

and $\mathrm{M}_d^{23} = -\mathrm{M}_d^{32} = \gamma$, where $2\xi_d^{\mp} = [i(1-2\langle n_{d\downarrow}\rangle)\langle j_{d\downarrow}^{\mp}\rangle + \langle i[n_{d\downarrow}, j_{d\downarrow}^{\mp}](1-2n_{d\uparrow})\rangle]/[\langle(\delta j_{d\downarrow}^{\mp})^2\rangle^{1/2}\langle(\delta n_{d\downarrow})^2\rangle^{1/2}]$ and $\gamma = -2i\sum_k V_{kd}^*\langle j_{d\downarrow}^- j_{d\downarrow}^+ c_{k\uparrow} c_{d\uparrow}^\dagger\rangle/[\langle(\delta j_{d\downarrow}^-)^2\rangle\langle(\delta j_{d\downarrow}^+)^2\rangle]^{1/2}$. These factors will be determined when we calculate the spectral densities.

In order to handle the infinite dimensional matrix, matrix reduction by Löwdin's partitioning technique[7] is performed by solving the eigenvalue equation for the original matrix $\mathbf{M}_{\mathrm{SIAM}}$, such as $\mathbf{M}_{\mathrm{SIAM}}\mathbf{C} = \mathbf{0}$, where $\mathbf{C}$ and $\mathbf{0}$ are infinite dimensional column vectors. The column vector $\mathbf{C}$ is partitioned into two parts, i.e., infinite dimensional $\mathbf{C}_r$ and three dimensional $\mathbf{C}_d$, symbolizing the reservoir and impurity parts, respectively. Then, the equation for $\mathbf{C}_d$ is obtained as $(\mathbf{M}_d - \mathbf{M}_{rd}\mathbf{M}_d^{-1}\mathbf{M}_{dr})\mathbf{C}_d \equiv \widetilde{\mathbf{M}}_d\mathbf{C}_d = \mathbf{0}$. The reduced 3×3 matrix $\widetilde{\mathbf{M}}_d$ contains the information on the many-body dynamics of a spin-up electron starting from the impurity site at $t = 0$ and ending at it at time t.

It is impossible to calculate the inverse of a general $\infty\times\infty$ matrix; however, this is not the case for the matrix $\mathbf{M}_r$, which is block diagonal. The inverse of $\mathbf{M}_r$ can be obtained in a straightforward manner[8]. The second term appears as additional self-energy terms in $\widetilde{\mathbf{M}}_d$ after reduction. One can easily imagine that $\xi_d^- = \xi_d^+$ in the Kondo regime at half-filling, and the final form of $\widetilde{\mathbf{M}}_d$ for a symmetric Anderson model in which $\epsilon_d = -U/2$ and $\langle n_d\rangle = 1/2$ is given by

$$\widetilde{\mathbf{M}}_d = \begin{pmatrix} -i\omega + i\Sigma_0 & U\xi_d^-/2 & U\xi_d^-/2 \\ -U\xi_d^-/2 & -i\omega + i\xi_d^{-2}\Sigma_0 & \gamma + i\xi_d^{-2}\Sigma_0 \\ -U\xi_d^-/2 & -\gamma + i\xi_d^{-2}\Sigma_0 & -i\omega + i\xi_d^{-2}\Sigma_0 \end{pmatrix},$$

where $\Sigma_0 = \sum_{\mathbf{k}} |V_{kd}|^2/(\omega - \epsilon_{\mathbf{k}} + i\eta) \equiv \Lambda(\omega) - i\Delta(\omega)$ is the self-energy of the Anderson model with $U = 0$. We will neglect the $\mathbf{k}$ dependence of V_{kd} in this work. The real and imaginary parts are respectively $\Lambda(\omega) = (\mathrm{P}/\pi)\int_{-\infty}^{\infty}\Delta(\epsilon)d\epsilon/(\omega-\epsilon)$, where P represents the principal integration and $\Delta(\omega) = \pi\sum_k |V_{kd}|^2\delta(\omega - \epsilon_{\mathbf{k}}) = \Delta[1-(\omega/D)^2]^{1/2}$ for the semielliptical band, where $\Delta = 2|V|^2/D$ and D is half of the band width. Now, one can obtain the retarded Green's function that is given by $iG_{dd}^+(\omega) = (\mathrm{adj}\ \widetilde{\mathbf{M}}_d)_{11}[\det\widetilde{\mathbf{M}}_d]^{-1}$ by calculating the inverse of matrix $\widetilde{\mathbf{M}}_d$.

We find that γ determines the width of the Kondo peak, while ξ_d^- governs the spacing of the side-peaks of the spectral density. Therefore, from the analysis at atomic limit, one can find that $\xi_d^- = 1/\sqrt{2}$. On the other hand, our retarded Green's function gives the real and imaginary parts of the self-energy as $\mathrm{Re}\Sigma_{\uparrow U}^+(\omega) = -(U^2/4\gamma^2)\omega + O(\omega^3)$ and $(1/\Delta)\mathrm{Im}\Sigma_{\uparrow U}^+(\omega) = (U^2/2\gamma^4)\omega^2 + O(\omega^4)$. The subscript U indicates the interaction part of the self-energy. The real part of the self-energy provides the wavefunction renormalization as $Z = 1/[1 + (U^2/4\gamma^2)]$.

FIG. 2: Spectral densities of the symmetric Anderson model with various Coulomb repulsions.

Unfortunately, it is difficult to obtain γ by direct calculation. Therefore, we determine rigorous γ by using the result of Bethe ansatz, which is given by $Z^{BA} = (4/\pi)\sqrt{U/\Gamma}\exp[-\pi U/4\Gamma + \pi\Gamma/4U]$ for the symmetric Anderson model[3]. We plot the spectral density $\rho_{d\uparrow}(\omega) = -(1/\pi)\mathrm{Im}G_{dd}^+(\omega)$ in Fig. 2. Our result naturally compatible with that of NRG at least in the Kondo regime.

The above result can be extended to nonequilibrium transport in a lead-dot-lead system with on-site Coulomb interaction at the dot in a straightforward manner because it is simply a single-impurity Anderson model with two separate metallic reservoirs. This only necessitates the simple requirement of an additional number of bases for describing the left and right leads and the movements from or to both leads, such as S_k^L, S_n^L for the left lead, $S_d^{\ell d\ell} \equiv \{\delta j_{d\downarrow}^{-L} c_{d\uparrow}, \delta j_{d\downarrow}^{+L} c_{d\uparrow}, c_{d\uparrow}, \delta j_{d\downarrow}^{-R} c_{d\uparrow}, \delta j_{d\downarrow}^{+R} c_{d\uparrow}\}$ for the dot, and S_k^R, S_n^R for the right lead. The superscripts L and R denote the left and right leads, respectively.

If we arrange S_k^L, S_n^L, $S_d^{\ell d\ell}$, S_k^R, S_n^R in a regular sequence to construct the matrix $\mathbf{M}$ for a lead-dot-lead system, it will be represented by a matrix of nine blocks,

$$\mathbf{M}_{\ell d\ell} = \begin{pmatrix} \mathbf{M}_{LL} & \mathbf{M}_{dL} & \mathbf{0} \\ \mathbf{M}_{Ld} & \mathbf{M}_d & \mathbf{M}_{Rd} \\ \mathbf{0} & \mathbf{M}_{dR} & \mathbf{M}_{RR} \end{pmatrix},$$

where blocks M_d, M_{dL} and M_{dR}, and M_{Ld} and M_{Rd} are 5×5, $5\times\infty$, and $\infty\times 5$ matrices, respectively. Blocks $\mathbf{M}_{LL}$ and $\mathbf{M}_{RR}$ are $\infty\times\infty$ matrices that are constructed by the sets of bases describing left and right leads, respectively. Since no direct coupling exists between the left and right leads, zero matrices are present at two of the corners. The structure of each block is similar to that of the corresponding block of the matrix $\mathbf{M}_{\mathrm{SIAM}}$.

The matrix reduction produces a 5×5 matrix for $\widetilde{\mathbf{M}}_d$, whose inverse yields the on-site retarded Green's function $G_{dd}^+(\omega)$ of the lead-dot-lead system in the framework of the NDT, which is given by a function of $\langle n_{d\sigma}\rangle$, $\langle j_{d\sigma}^{-L,R}\rangle$, $\langle j_{d\sigma}^{+L,R}\rangle$. Since the current is expressed by

$J_\sigma = J_\sigma^L = -J_\sigma^R = (J_\sigma^L - J_\sigma^R)/2$, where $J_\sigma^L = (e/\hbar)\langle j_{d\sigma}^{-L}\rangle$, the current and other variables are expressed by the lesser and retarded Green's functions such that[1, 4]

$$\begin{aligned}\langle j_{d\sigma}^{-L}\rangle &= \int \frac{d\omega}{\pi}\left\{i\Gamma_\sigma^L(\omega)G_{dd\sigma}^<(\omega)\right. \\ &- \left. 2f_L(\omega)\Gamma_\sigma^L(\omega)\mathrm{Im}G_{dd\sigma}^+(\omega)\right\} \qquad (1)\end{aligned}$$

$$\langle j_{d\sigma}^{+L}\rangle = \int \frac{d\omega}{\pi}[f_L(\omega)\Gamma_\sigma^L(\omega)\mathrm{Re}G_{dd\sigma}^+(\omega) - iG_{dd\sigma}^<(\omega)\Lambda(\omega)], \qquad (2)$$

$$\langle n_{d\sigma}\rangle = \frac{-i}{2\pi}\int d\omega G_{dd\sigma}^<(\omega) = \frac{-1}{\pi}\int d\omega \tilde{f}(\omega)\mathrm{Im}G_{dd\sigma}^+(\omega), \qquad (3)$$

where the effective Fermi distribution $\tilde{f}(\omega)$ is given by[9]

$$\tilde{f}(\omega) = \frac{f_L(\omega)\Gamma_\sigma^L(\omega) + f_R(\omega)\Gamma_\sigma^R(\omega) + \frac{1}{i}\Sigma_{\sigma U}^<(\omega)}{\Gamma_\sigma^L(\omega) + \Gamma_\sigma^R(\omega) - 2\mathrm{Im}\Sigma_{\sigma U}^+(\omega)}. \qquad (4)$$

In order to construct a self-consistent loop for calculating the current-voltage characteristics, we use the Keldysh equation[1]

$$G_\sigma^<(\omega) = G_\sigma^+(\omega)\Sigma_\sigma^<(\omega)G_\sigma^-(\omega). \qquad (5)$$

Then, one can construct a self-consistent loop from Eqs. (1)-(5) as

$\langle n_{d\sigma}\rangle^{(0)}, \langle j_{d\sigma}^{\mp}\rangle^{(0)} \to G_{dd\sigma}^{+(0)}(\omega) \to \tilde{f}_\sigma^{(0)}(\omega) \to G_{dd\sigma}^{<(0)}(\omega)$ $\to \langle n_{d\sigma}\rangle^{(1)}, \langle j_{d\sigma}^{\mp}\rangle^{(1)} \to G_{dd\sigma}^{+(1)}(\omega) \to \Sigma_{\sigma U}^{<(1)}(\omega) \to \tilde{f}_\sigma^{(1)}(\omega)$ $\to \cdots$.

This iterative method for calculating nonequilibrium quantities of the strongly correlated system is the second major result of this work. The specific results will be reported in a separate work.

This work was supported by Korea Research Foundation Grant No. KRF-2003-070-C00020.

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